General Considerations. All manipulations were carried out using either high-vacuum or glovebox techniques as described earlier.[2] ^1H and ^{13}C NMR NMR spectra were recorded on a GE 300 NMR spectrometer. Microanalyses were performed by Fenton Harvey of this department. Toluene and petroleum ether were distilled from benzophenone ketyl and then vacuum distilled from titanocene prior to use.[3] $HfCl_4$ (Aesar) was purified by sublimation (170°C at 10^{-3} torr) before further use and HCl (technical grade) was purchased from Matheson and used as received. The preparation of $Li_2[C_4H_4BN(CHMe_2)_2]\cdot THF$[4], Cp^*ZrCl_3[5] and Cp^*HfCl_3[6] were carried out as described.

Preparation of $Cp^*[C_4H_4BNCHMe_2)_2]ZrCl\cdot LiCl$ (1a). A 100 mL round bottom flask was charged with 2.50 g (7.51 mmoles) Cp^*ZrCl_3 and 1.87 g (7.51 mmoles) of $Li_2[C_4H_4BN(CHMe_2)_2]\cdot THF$. On a high vacuum line, approximately 60 mL toluene were condensed on the solids at -78°C. The resulting mixture was allowed to warm slowly to room temperature under vigorous stirring and was stirred an additional 24 hours. The reaction mixture was filtered and volatiles removed *in vacuo* to yield a purple solid which was washed with 20 mL of cold (-78°C) petroleum ether and refiltered to yieled $Cp^*[C_4H_4BN(CHMe_2)_2]ZrCl\cdot LiCl$ as a bright purple microcrystaline solid. (2.01 g, 57%). ^1H NMR (300 MHz, benzene-d_6/THF-d_8): δ -NCH-(CH_3)$_2$, 1.31 (d, 12H); [$C_5(CH_3)_5$], 2.00 (s, 15H); -NC*H*-(CH_3)$_2$, 3.74 (m, 2H); -B-CH-C*H*-, 4.48 (t, 2H); -B-C*H*-CH-, 5.77 (t, 2H). ^{13}C NMR (75 MHz benzene-d_6/THF-d_8): δ [$C_5(CH_3)_5$], 12.3; -NCH-(CH_3)$_2$, 24.0; -NCH-(CH_3)$_2$, 47.3; -B-CH-CH-, 97.7; [$C_5(CH_3)_5$], 119.7; -B-CH-CH-, 124.5. Anal. Calcd.: C, 56.53; H, 7.83; N, 3.30. Found: C, 53.15; H, 7.17; N, 2.71.

Preparation of $Cp^*[C_4H_4BNCHMe_2)_2]HfCl\cdot LiCl$ (1b). A swivel frit was charged with 1.0 g Cp^*HfCl_3 (2.38×10^{-3} mol) and 592 mg $Li_2(C_4H_4BN^iPr_2)(THF)$ (1 eq). On the vacuum line, 125 mL toluene were condensed in at -78°C, and the solution was allowed to gradually warm to ambient temperature and stirred an additional 8 hr. The red solution was filtered and the volatiles removed *in vacuo*. . Petroleum ether (50 mL) was condensed and the resulting red-orange slurry was stirred for two hours. The product was isolated by filtration and then washed with a small amount of petroleum ether. (830mg, 63%). ^1H NMR (300 MHz, THF-d_8) δ -NCH-(CH_3)$_2$, 1.06 (d, 12H); [$C_5(CH_3)_5$], 1.87 (s, 15H); -B-CH-C*H*-, 3.29 (m, 2H); -NC*H*-(CH_3)$_2$, 3.44 (septet, 2H); -B-C*H*-CH-, 5.05 (m, 2H). ^{13}C NMR (75 MHz THF-d_8): δ [$C_5(CH_3)_5$], 12.0; -NCH-

$(CH_3)_2$, 23.8; -NCH-$(CH_3)_2$, 47.0; -B-CH-CH_2, 87.3 ; -B-CH-CH-, 116.1; [$C_5(CH_3)_5$], 119.2. Anal. Calc. : C, 43.33; H, 6.31; N, 2.52. Found: C, 43.11; H, 5.98; N, 2.20.

Preparation of Cp*[$C_4H_4BNCHMe_2)_2$]$HfCl_2$ (2b). A swivel frit assembly was charged with 1.25 g Cp*[$C_4H_4BNCHMe_2)_2$]HfCl·LiCl ($2.26x10^{-3}$ mol) and 50 mL of ether were condensed in at -78°C on the high vacuum line. Using a 104 mL gas bulb, 402 torr HCl (1 eq) was condensed in at -78°C. Upon warming to ambient temperature, the blue-purple solution rapidly turned yellow. The solution was stirred an additional two hours befor the volatiles were removed *in vacuo*.. Toluene (50 mL) was condensed in, the solution filtered, and volatiles removed. Petroleum ether (40mL) was condensed onto the residue, and a yellow solid was isolated on the frit by cold filtration. (0.96g 78%). ^{1}H NMR (300 MHz, benzene-d_6): δ -NCH-(CH_3)$_2$, 0.92(d, 6H); -NCH-(CH_3)$_2$, 0.97 (d, 6H); [$C_5(CH_3)_5$], 2.15 (s, 15H); -NC*H*-$(CH_3)_2$, 3.25 (septet, 2H); -B-CH-C*H*-, 4.75 (m, 2H); -B-C*H*-CH-, 5.90 (m, 2H); -N*H*CH-$(CH_3)_2$, 6.38 (br, 1H). ^{13}C NMR (75 MHz benzene-d_6): δ [$C_5(CH_3)_5$], 12.1; -NCH-$(CH_3)_2$, 19.4; -NCH-$(CH_3)_2$, 20.2; -NCH-$(CH_3)_2$, 50.6; -B-CH-CH-, 114.3 (C α to B not located); [$C_5(CH_3)_5$], 119.1. Anal. Calc.: C, 43.80; H, 6.20; N, 2.55. Found: C, 42.80; H, 6.06; N, 2.37.

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1. Present address: Department of Chemistry, University of Rochester, Rochester, NY 14627.
2. Burger, B.J.; Bercaw, J. E. In *Experimental Organometallic Chemistry*; Wayda, A.L., Darensbourg, M. Y. Eds.; ACS Symposium Series 357; American Chemical Society, Washington, D. C. 1987.
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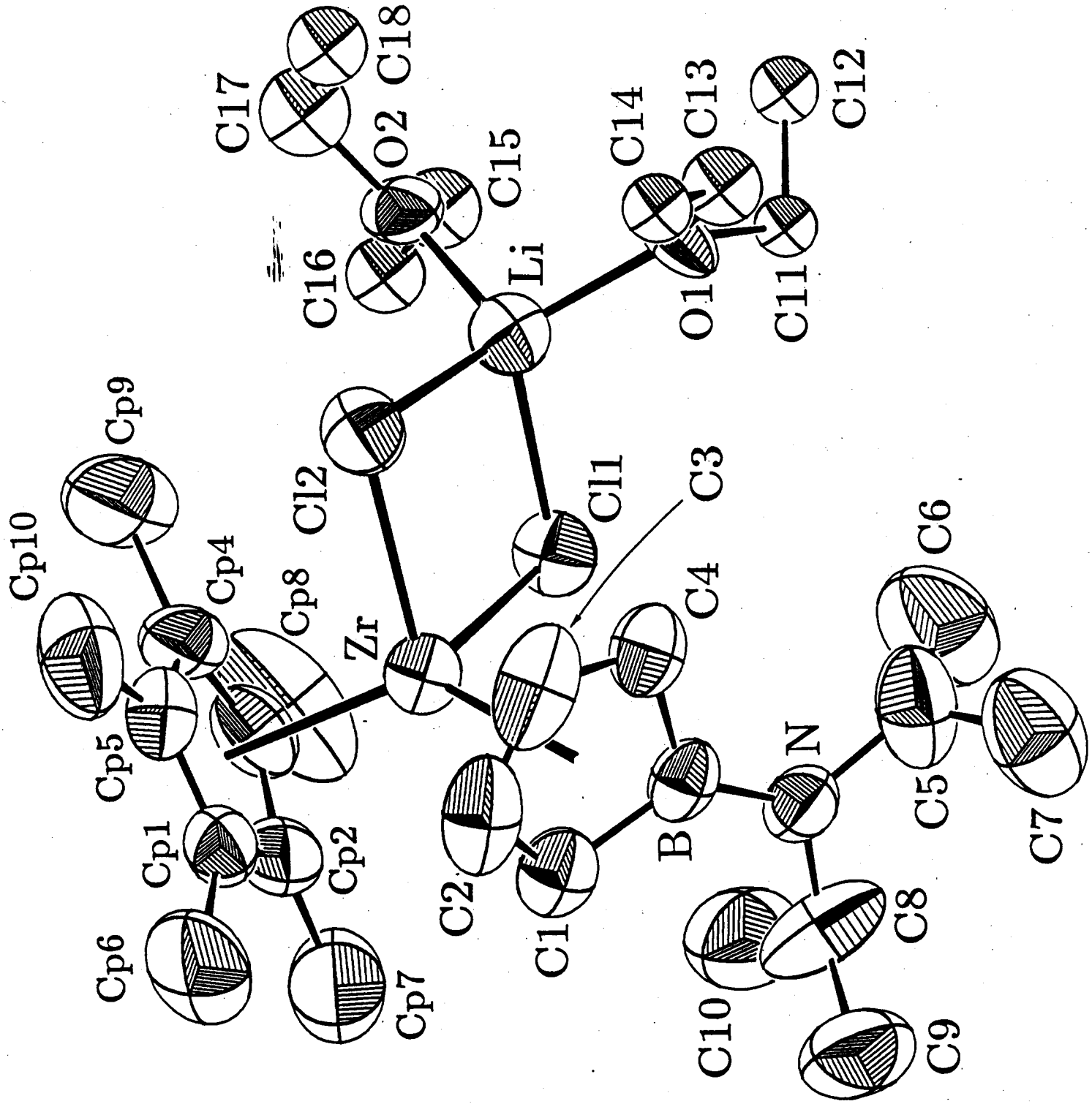

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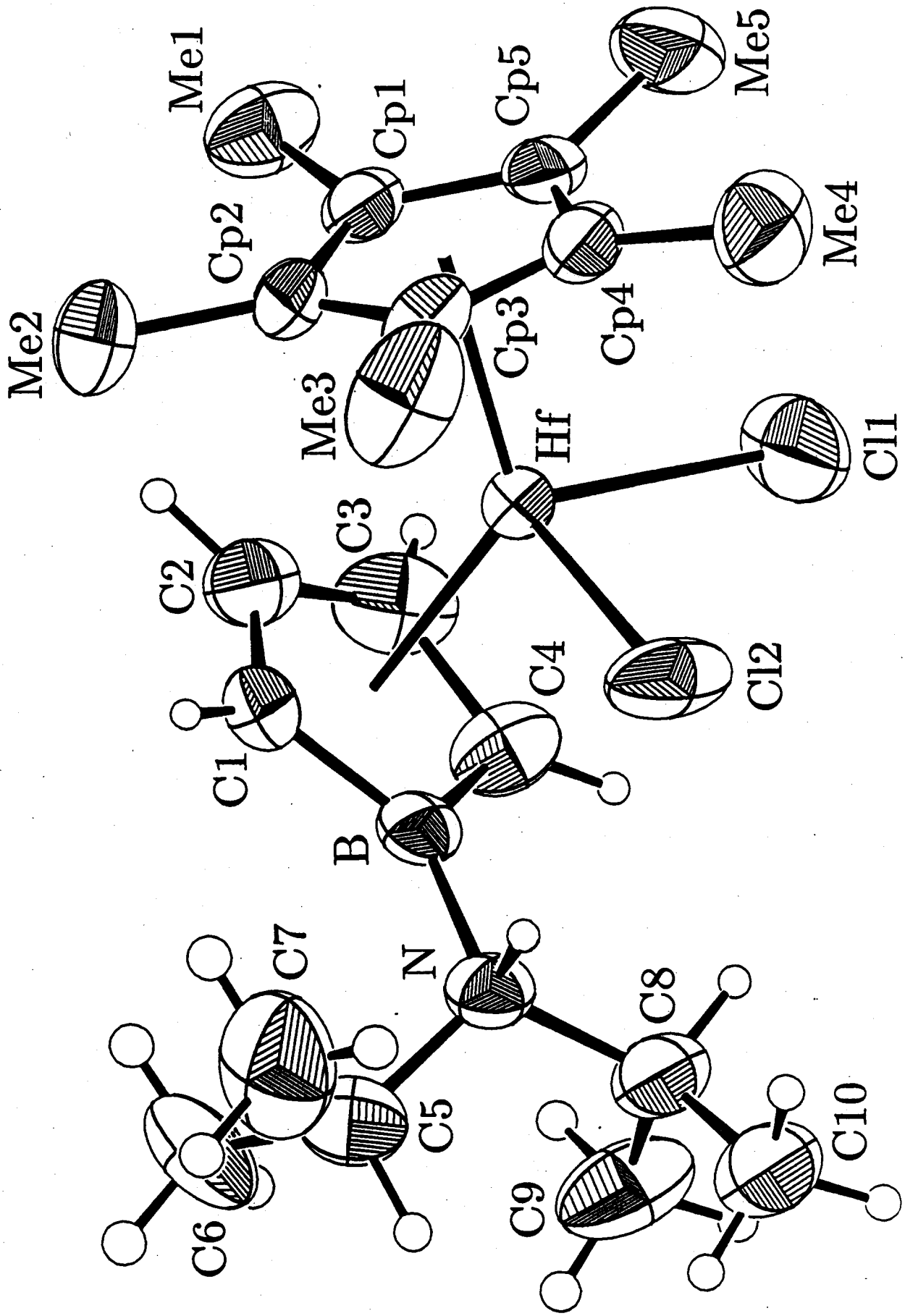

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X-ray I.D. RWQ10

Name of Compound Cp^* Zr Cl Complex · Li Diethérate

Chemical Formula $C_{28}H_{53}BCl_2NO_2ZrLi$ M. wt. 615.61

Crystal System MONOCLINIC Space Group $P2_1/n$ (# 14)

a=	11.013(5)	Å	α=	90	
b=	21.440(11)	Å	β=	95.91(3)°	
c=	14.462(5)	Å	γ=	90	
V=	3396.6(26)	Å^3	Z=	4	
D_m	—	g cm^{-3}	D_x	1.20	g cm^{-3}

Radiation used MoKα Wavelength 0.71073 Å

Absorption Coefficient, μ= 4.98 cm^{-1} Temperature 295 °K

Type of Absorption Correction none used (program used) _____

$\mu r_{max} = 0.30$

Range of Transmission Factors _____

Crystal Color blue Crystal Shape (Habit) plate

Crystal Size 0.11 mm × 0.30 mm × 1.15 mm

Source of Crystal RWQ

Type of Diffractometer Enraf-Nonius Cad-4

Data Collection method (diffraction geometry, scan type) omega scans

Lattice Parameters: Number of reflections 25; θ range ~~11° to 13.2°~~ 16° to 18°

θ range for data collection 1° to 21°

h_{min} -11 h_{max} 0 k_{min} -23 k_{max} 23 l_{min} -15 l_{max} 15

Number of reflections measured 7997

Number of independent reflections 3714

Number of reflections used in refinement 3714

Criterion for reflections used all used, F_o^2 positive and negative

Goodness of fit for merging data 1.00 (number of multiples 3581)

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R_{int} for duplicate reflections 0.036 (number of duplicates 2711)

Number of standard reflections 3 Interval 150 minutes

Variations of standards linear decay of 1.6% during data collection: corrected for

How structure solved? Zr atom coordinates found from Patterson, remaining heavy atoms found from successive structure factor - Fourier cycles.

How H atoms treated? positioned by calculation (C-H, 0.95 Å) or, for CH_3 groups, at idealized positions based on difference maps calculated in the expected planes. Re-positioned prior to final refinement cycles.

Refinement on F^2, $w=1/\sigma^2(F_o^2)$, one full matrix used.

R = 0.080 on F for 3351 reflections with $F_o^2 > 0$

R = 0.054 on F for 2421 reflections with $F_o^2 > 3\sigma(F_o^2)$

wR = 0.012 on F^2 for 3714 reflections

Goodness of Fit (S) = 2.44 for 3714 data and 286 parameters

$(\Delta/\sigma)_{max}$ in final least squares cycle 0.12

$\Delta\rho_{max}$ +0.88 eÅ^{-3}, $\Delta\rho_{min}$ -0.65 eÅ^{-3} in final difference map. all big peaks near ether molecules

Secondary Extinction parameter (if used) 0.38(4) x10^{-6}

(Reference: Larson, A. C. (1967). *Acta Cryst.* 23, 644-665.)

Computer Programs

The CRYM Crystallographic Computing System

(Duchamp, D. J. (1964). Am. Crystallogr. Assoc. Meet., Bozeman, Montana, Paper B14, p. 29.)

ORTEP

(Johnson, C. K. (1976). *ORTEP*II. Report ORNL-3794. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.)

MULTAN88

Debaerdemaeker, T., Germain, G., Main, P., Refaat, L. S., Tate, C. & Woolfson, M. M. (1988). *MULTAN 88. Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*, Univs. of York, England and Louvain, Belgium.

Scattering Factors and f', f'':

Cromer, D. T. (1974). *International Tables For X-ray Crystallography*, Vol. IV, pp. 149–151. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Cromer, D. T. & Waber, J. T. (1974). *International Tables For X-ray Crystallography*, Vol. IV, pp. 99–101. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Any additional Data:

Weights w are calculated as $1/\sigma^2(F_o^2)$; variances ($\sigma^2(F_o^2)$) were derived from counting statistics plus an additional term, $(0.014I)^2$; variances of the merged data were obtained by propagation of error plus another additional term, $(0.014\bar{I})^2$.

Definitions:

$$R = \frac{\Sigma||F_o| - |F_c||}{\Sigma F_o}; \quad R_w = \frac{\Sigma w(F_o^2 - F_c^2)}{\Sigma w F_o^2}$$

$$S = \left\{ \frac{\Sigma w(F_o^2 - F_c^2)^2}{n-p} \right\}^{\frac{1}{2}}$$

where n = number of data,

p = number of parameters refined.

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Table 1. Final Refined Parameters for Zirconium Cp*, C_4B-Ring Chloride, LiCl Dietherate.

x, y, z and $U_{eq}{}^a \times 10^4$

Atom	x	y	z	U_{eq} or B
Zr	2170(.7)	2008(.3)	4209(.4)	533(2)
Cl1	672(2)	2046(1)	2760(1)	637(5)
Cl2	1212(2)	958(1)	4571(1)	686(6)
Cp1	4481(7)	2048(5)	4480(6)	674(25)
Cp2	4172(8)	2310(4)	3607(7)	746(28)
Cp3	3687(7)	1841(5)	3013(5)	706(27)
Cp4	3654(7)	1298(4)	3518(7)	740(27)
Cp5	4157(7)	1423(4)	4437(6)	646(25)
Cp6	5267(9)	2364(5)	5283(7)	1327(38)
Cp7	4521(9)	2948(5)	3305(8)	1394(39)
Cp8	3365(9)	1913(6)	1972(6)	1513(47)
Cp9	3318(9)	648(5)	3155(7)	1384(39)
Cp10	4355(8)	945(5)	5202(7)	1144(33)
C1	2313(7)	3022(4)	4924(5)	665(23)
C2	2481(9)	2563(5)	5618(6)	878(33)
C3	1397(11)	2255(4)	5687(6)	862(34)
C4	466(7)	2478(4)	5013(5)	667(23)
B	956(8)	3063(4)	4589(5)	544(25)
N	308(6)	3512(3)	3991(4)	599(19)
C5	−1002(10)	3498(4)	3810(7)	1003(34)

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Table 1. (Cont.)

Atom	x	y	z	U_{eq} or B
C6	−1551(9)	3341(5)	2886(7)	1392(41)
C7	−1699(9)	3871(5)	4417(6)	1243(36)
C8	876(11)	4046(4)	3621(7)	1103(40)
C9	1301(9)	4540(4)	4244(7)	1201(35)
C10	1500(10)	3920(5)	2802(8)	1289(39)
Li	−258(12)	1107(6)	3240(9)	737(40)
O1	−1956(5)	1212(3)	3426(4)	1191(23)
C11	−2729(12)	1520(6)	2645(9)	11.7(3) *
C12	−3458(12)	1070(6)	2120(9)	13.8(4) *
C13	−2589(16)	1095(8)	4145(14)	19.3(6) *
C14	−2060(13)	934(6)	4978(10)	14.7(4) *
O2	−182(6)	436(3)	2306(5)	1179(23)
C15	−394(19)	604(9)	1282(15)	20.5(8) *
C16	361(17)	724(8)	897(12)	18.1(6) *
C17	−84(22)	−197(12)	2488(15)	24.6(9) *
C18	−622(17)	−404(8)	3015(13)	18.8(6) *

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

* Isotropic displacement parameter, B

Table 2. Assigned Hydrogen Atom Parameters for Zirconium Cp*, C_4B-Ring Chloride, LiCl Dietherate.

x, y and $z \times 10^4$

Atom	x	y	z	B
HM1A	6096	2340	5167	12.1
HM1B	5146	2149	5844	12.1
HM1C	5017	2785	5321	12.1
HM2A	3888	3095	2856	12.4
HM2B	5264	2917	3035	12.4
HM2C	4600	3213	3829	12.4
HM3A	3206	2343	1841	13.7
HM3B	2661	1671	1791	13.7
HM3C	4035	1775	1664	13.7
HM4A	2590	526	3378	12.6
HM4B	3972	376	3359	12.6
HM4C	3232	669	2489	12.6
HM5A	4844	1124	5711	10.3
HM5B	4751	592	4972	10.3
HM5C	3580	827	5385	10.3
H1	2943	3268	4702	5.9
H2	3228	2475	5986	8.0
H3	1284	1935	6128	7.8
H4	−319	2295	4863	6.0
H5	−1161	3098	4062	9.1
H6A	−983	3097	2591	12.6
H6B	−2268	3105	2941	12.6
H6C	−1737	3710	2554	12.6
H7A	−1217	3930	4990	11.2
H7B	−1891	4256	4128	11.2
H7C	−2423	3651	4515	11.2
H8	175	4272	3365	10.1
H9A	798	4560	4739	10.8
H9B	2115	4460	4479	10.8
H9C	1248	4923	3911	10.8
H10A	1112	3588	2471	11.5

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Table 2. (Cont.)

Atom	x	y	z	B
H10B	1455	4288	2429	11.5
H10C	2322	3826	2997	11.5
H11A	−3247	1816	2894	13.5
H11B	−2216	1723	2253	13.5
H12A	−3934	1282	1633	15.8
H12B	−2938	779	1872	15.8
H12C	−3969	872	2514	15.8
H13A	−2973	1494	4253	22.4
H13B	−3176	806	3945	22.4
H14A	−2685	880	5375	17.1
H14B	−1688	530	4895	17.1
H14C	−1484	1219	5203	17.1
H15A	−718	201	1016	16.0
H15B	−1027	887	1242	16.0
H16A	−24	797	274	15.8
H16B	626	1118	1151	15.8
H16C	935	432	924	15.8
H17A	−461	−382	1886	28.8
H17B	727	−293	2548	28.8
H18A	−428	−838	3016	20.9
H18B	−221	−227	3587	20.9
H18C	−1409	−316	2924	20.9

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Table 3. Anisotropic Displacement Parameters for Zirconium Cp*, C_4B-Ring Chloride, LiCl Dietherate.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zr	606(5)	574(5)	417(4)	42(5)	46(3)	−6(5)
Cl1	689(13)	706(13)	501(11)	17(13)	−8(10)	58(11)
Cl2	669(15)	711(14)	680(14)	21(12)	81(11)	166(11)
Cp1	533(51)	689(64)	774(63)	70(53)	−64(44)	−169(58)
Cp2	594(61)	643(61)	1017(77)	−69(50)	166(56)	178(62)
Cp3	540(56)	1012(81)	574(57)	−14(54)	92(45)	44(58)
Cp4	643(61)	729(67)	880(72)	−125(51)	230(55)	−393(59)
Cp5	628(58)	656(62)	657(63)	162(49)	87(48)	59(50)
Cp6	945(79)	1600(94)	1330(89)	130(69)	−399(69)	−720(73)
Cp7	987(78)	1039(78)	2216(117)	141(74)	455(79)	414(85)
Cp8	949(75)	3052(146)	562(58)	−47(93)	192(54)	167(83)
Cp9	1005(82)	1312(89)	1921(108)	−257(68)	560(78)	−1024(80)
Cp10	855(72)	1309(82)	1267(82)	351(64)	107(64)	427(68)
C1	800(62)	660(52)	518(48)	105(54)	−12(43)	−89(47)
C2	1040(87)	1044(79)	519(62)	436(68)	−62(62)	−166(56)
C3	1357(98)	900(75)	376(52)	432(69)	308(63)	94(46)
C4	756(63)	680(58)	592(53)	146(50)	202(50)	−78(45)
B	701(69)	495(62)	433(50)	116(61)	37(49)	−105(52)
N	672(51)	465(42)	639(43)	42(38)	−40(38)	−5(34)
C5	869(81)	1283(87)	820(71)	404(69)	−90(63)	−150(62)
C6	1078(89)	1883(113)	1176(88)	−62(78)	−73(74)	−587(77)
C7	952(77)	1749(102)	1038(78)	171(75)	153(65)	−343(72)
C8	1929(117)	547(63)	839(75)	−111(72)	165(75)	−142(58)
C9	1306(91)	857(71)	1479(91)	−216(66)	335(75)	−417(68)
C10	1323(97)	1090(85)	1507(103)	−194(73)	406(82)	−49(74)
Li	664(98)	659(92)	870(100)	18(76)	−13(82)	−49(78)
O1	791(47)	1721(64)	1068(51)	−180(44)	134(41)	459(47)
O2	1215(56)	937(49)	1326(59)	−148(42)	−150(46)	243(43)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*^2} + U_{22}k^2b^{*^2} + U_{33}\ell^2c^{*^2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

Table 4. Complete Distances and Angles for Zirconium Cp*, C_4B-Ring Chloride, LiCl Dietherate.

		Distance(Å)			Distance(Å)
Zr	–Cl1	2.531(2)	N	–C8	1.434(12)
Zr	–Cl2	2.563(2)	C5	–C6	1.448(14)
Zr	–Cp	2.236	C5	–C7	1.463(14)
Zr	–Cp1	2.535(8)	C8	–C9	1.437(14)
Zr	–Cp2	2.536(9)	C8	–C10	1.454(14)
Zr	–Cp3	2.550(9)	O1	–C11	1.496(14)
Zr	–Cp4	2.515(9)	O1	–C13	1.334(19)
Zr	–Cp5	2.514(8)	C11	–C12	1.423(18)
Zr	–Cb	2.165	C13	–C14	1.33(2)
Zr	–C1	2.405(8)	O2	–C15	1.52(2)
Zr	–C2	2.354(10)	O2	–C17	1.38(3)
Zr	–C3	2.439(10)	C15	–C16	1.08(3)
Zr	–C4	2.518(8)	C17	–C18	1.10(3)
Zr	–B	2.714(9)	Cp6	–Hp1A	0.946
Li	–Cl1	2.393(13)	Cp6	–Hp1B	0.955
Li	–Cl2	2.405(13)	Cp6	–Hp1C	0.948
Li	–O1	1.930(14)	Cp7	–Hp2A	0.956
Li	–O2	1.982(15)	Cp7	–Hp2B	0.945
Cp1	–Cp2	1.390(12)	Cp7	–Hp2C	0.944
Cp1	–Cp5	1.387(12)	Cp8	–Hp3A	0.954
Cp1	–Cp6	1.533(13)	Cp8	–Hp3B	0.947
Cp2	–Cp3	1.393(13)	Cp8	–Hp3C	0.947
Cp2	–Cp7	1.497(14)	Cp9	–Hp4A	0.932
Cp3	–Cp4	1.376(12)	Cp9	–Hp4B	0.951
Cp3	–Cp8	1.520(13)	Cp9	–Hp4C	0.959
Cp4	–Cp5	1.412(12)	Cp10	–Hp5A	0.948
Cp4	–Cp9	1.520(13)	Cp10	–Hp5B	0.949
Cp5	–Cp10	1.508(13)	Cp10	–Hp5C	0.954
C1	–C2	1.404(12)	C1	–H1	0.952
C1	–B	1.526(12)	C2	–H2	0.952
C2	–C3	1.377(14)	C3	–H3	0.953
C3	–C4	1.423(12)	C4	–H4	0.954
C4	–B	1.520(12)	C5	–H5	0.955
B	–N	1.433(11)	C6	–H6A	0.949
N	–C5	1.440(11)	C6	–H6B	0.949

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Table 4. (Cont.)

Distance(Å)			Angle(°)			
C6	–H6C	0.937	Cl1	–Zr	–Cl2	87.1(1)
C7	–H7A	0.945	Cp	–Zr	–Cb	132.7
C7	–H7B	0.940	Cp	–Zr	–Cl1	109.3
C7	–H7C	0.950	Cp	–Zr	–Cl2	105.8
C8	–H8	0.954	Cb	–Zr	–Cl1	106.2
C9	–H9A	0.950	Cb	–Zr	–Cl2	106.3
C9	–H9B	0.941	Cl1	–Li	–Cl2	94.1(5)
C9	–H9C	0.951	Cl1	–Li	–O1	113.1(6)
C10	–H10A	0.937	Cl1	–Li	–O2	111.3(6)
C10	–H10B	0.954	Cl2	–Li	–O1	119.1(6)
C10	–H10C	0.942	Cl2	–Li	–O2	112.1(6)
C11	–H11A	0.949	O1	–Li	–O2	106.8(7)
C11	–H11B	0.947	Zr	–Cl1	–Li	89.7(3)
C12	–H12A	0.949	Zr	–Cl2	–Li	88.7(3)
C12	–H12B	0.942	Cp5	–Cp1	–Cp2	108.2(8)
C12	–H12C	0.942	Cp6	–Cp1	–Cp2	125.2(8)
C13	–H13A	0.975	Cp6	–Cp1	–Cp5	125.7(8)
C13	–H13B	0.920	Cp3	–Cp2	–Cp1	108.1(8)
C14	–H14A	0.947	Cp7	–Cp2	–Cp1	125.9(8)
C14	–H14B	0.970	Cp7	–Cp2	–Cp3	125.0(8)
C14	–H14C	0.916	Cp4	–Cp3	–Cp2	108.3(8)
C15	–H15A	0.997	Cp8	–Cp3	–Cp2	125.0(8)
C15	–H15B	0.920	Cp8	–Cp3	–Cp4	126.5(8)
C15	–H16B	1.598	Cp5	–Cp4	–Cp3	108.0(8)
C16	–H16A	0.969	Cp9	–Cp4	–Cp3	127.6(8)
C16	–H16B	0.954	Cp9	–Cp4	–Cp5	123.9(8)
C16	–H16C	0.888	Cp4	–Cp5	–Cp1	107.5(7)
C17	–H17A	1.007	Cp10	–Cp5	–Cp1	127.4(8)
C17	–H17B	0.911	Cp10	–Cp5	–Cp4	125.1(8)
C18	–H18A	0.955	B	–C1	–C2	108.7(7)
C18	–H18B	0.973	C3	–C2	–C1	109.7(8)
C18	–H18C	0.883	C4	–C3	–C2	111.0(8)
			B	–C4	–C3	107.0(7)
			C4	–B	–C1	101.6(7)
			N	–B	–C1	129.9(7)

Table 4. (Cont.)

			Angle(°)				Angle(°)
N	–B	–C4	128.5(7)	Hp4B	–Cp9	–Cp4	107.8
C5	–N	–B	121.6(7)	Hp4C	–Cp9	–Cp4	107.5
C8	–N	–B	123.5(7)	Hp4B	–Cp9	–Hp4A	111.8
C8	–N	–C5	114.6(7)	Hp4C	–Cp9	–Hp4A	111.2
C6	–C5	–N	119.2(8)	Hp4C	–Cp9	–Hp4B	109.5
C7	–C5	–N	117.2(8)	Hp5A	–Cp10	–Cp5	108.7
C7	–C5	–C6	119.1(9)	Hp5B	–Cp10	–Cp5	108.8
C9	–C8	–N	118.7(8)	Hp5C	–Cp10	–Cp5	108.5
C10	–C8	–N	114.6(8)	Hp5B	–Cp10	–Hp5A	110.6
C10	–C8	–C9	119.8(9)	Hp5C	–Cp10	–Hp5A	110.2
C13	–O1	–C11	111.7(10)	Hp5C	–Cp10	–Hp5B	110.0
C12	–C11	–O1	110.4(10)	H1	–C1	–C2	125.6
C14	–C13	–O1	122.7(15)	H1	–C1	–B	125.8
C17	–O2	–C15	114.8(13)	H2	–C2	–C1	125.5
C16	–C15	–O2	120.7(19)	H2	–C2	–C3	124.8
C18	–C17	–O2	119.1(22)	H3	–C3	–C2	124.6
Hp1A	–Cp6	–Cp1	108.8	H3	–C3	–C4	124.4
Hp1B	–Cp6	–Cp1	108.3	H4	–C4	–C3	126.2
Hp1C	–Cp6	–Cp1	108.7	H4	–C4	–B	126.8
Hp1B	–Cp6	–Hp1A	110.2	H5	–C5	–N	99.7
Hp1C	–Cp6	–Hp1A	110.7	H5	–C5	–C6	93.9
Hp1C	–Cp6	–Hp1B	110.1	H5	–C5	–C7	97.7
Hp2A	–Cp7	–Cp2	108.0	H6A	–C6	–C5	108.1
Hp2B	–Cp7	–Cp2	108.4	H6B	–C6	–C5	108.6
Hp2C	–Cp7	–Cp2	108.7	H6C	–C6	–C5	108.9
Hp2B	–Cp7	–Hp2A	110.1	H6B	–C6	–H6A	109.7
Hp2C	–Cp7	–Hp2A	110.3	H6C	–C6	–H6A	110.7
Hp2C	–Cp7	–Hp2B	111.2	H6C	–C6	–H6B	110.7
Hp3A	–Cp8	–Cp3	108.4	H7A	–C7	–C5	108.5
Hp3B	–Cp8	–Cp3	108.6	H7B	–C7	–C5	108.8
Hp3C	–Cp8	–Cp3	108.7	H7C	–C7	–C5	108.6
Hp3B	–Cp8	–Hp3A	110.2	H7B	–C7	–H7A	110.7
Hp3C	–Cp8	–Hp3A	110.1	H7C	–C7	–H7A	109.9
Hp3C	–Cp8	–Hp3B	110.8	H7C	–C7	–H7B	110.3
Hp4A	–Cp9	–Cp4	109.0	H8	–C8	–N	100.6

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Table 4. (Cont.)

	Angle(°)		Angle(°)
H8 –C8 –C9	93.8	H14C –C14 –H14B	110.7
H8 –C8 –C10	102.1	H15A –C15 –O2	100.5
H9A –C9 –C8	109.2	H15B –C15 –O2	104.8
H9B –C9 –C8	109.2	H16B –C15 –O2	103.9
H9C –C9 –C8	108.7	H15A –C15 –C16	105.8
H9B –C9 –H9A	110.2	H15B –C15 –C16	115.5
H9C –C9 –H9A	109.4	H16B –C15 –C16	35.5
H9C –C9 –H9B	110.1	H15B –C15 –H15A	107.9
H10A –C10 –C8	109.2	H16B –C15 –H15A	141.2
H10B –C10 –C8	107.8	H16B –C15 –H15B	94.4
H10C –C10 –C8	108.5	H16A –C16 –C15	103.4
H10B –C10 –H10A	110.2	H16B –C16 –C15	103.6
H10C –C10 –H10A	111.3	H16C –C16 –C15	113.2
H10C –C10 –H10B	109.8	H16B –C16 –H16A	107.6
H11A –C11 –O1	109.1	H16C –C16 –H16A	113.3
H11B –C11 –O1	109.1	H16C –C16 –H16B	114.8
H11A –C11 –C12	109.1	H17A –C17 –O2	101.7
H11B –C11 –C12	109.3	H17B –C17 –O2	107.2
H11B –C11 –H11A	109.9	H17A –C17 –C18	103.7
H12A –C12 –C11	108.1	H17B –C17 –C18	115.8
H12B –C12 –C11	108.7	H17B –C17 –H17A	107.9
H12C –C12 –C11	108.8	H18A –C18 –C17	104.8
H12B –C12 –H12A	110.2	H18B –C18 –C17	101.6
H12C –C12 –H12A	110.2	H18C –C18 –C17	113.6
H12C –C12 –H12B	110.8	H18B –C18 –H18A	107.2
H13A –C13 –O1	103.3	H18C –C18 –H18A	115.1
H13B –C13 –O1	106.7	H18C –C18 –H18B	113.3
H13A –C13 –C14	103.9		
H13B –C13 –C14	109.7		
H13B –C13 –H13A	109.9		
H14A –C14 –C13	107.7		
H14B –C14 –C13	105.7		
H14C –C14 –C13	111.7		
H14B –C14 –H14A	108.1		
H14C –C14 –H14A	112.7		

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Table 5. Intermolecular Distances Less Than 3.5Åfor Zirconium Cp*, C_4B-Ring Chloride, LiCl Dietherate.

	Distance(Å)		Distance(Å)
Cl1 –Hp1B	3.266	C10 –Hp5A	3.369
Cl2 –H14B	3.312	C11 –H2	3.468
Cl2 –H18B	3.368	C12 –Hp3C	3.157
Cp1 –H13A	3.094	C13 –Hp1A	3.442
Cp2 –H11A	3.297	C13 –Hp5B	3.450
Cp3 –H11A	3.398	C14 –H18B	3.441
Cp3 –H12C	3.447	C16 –Hp1C	3.314
Cp4 –H12C	3.252	C16 –H15A	3.460
Cp5 –H13A	3.203	Hp1A –H7C	3.432
Cp5 –H13B	3.364	Hp1A –H13A	2.522
Cp6 –H13A	3.169	Hp1A –H14A	3.407
Cp6 –H16B	3.497	Hp1A –Hp3A	3.250
Cp7 –H18A	3.438	Hp1A –Hp3B	3.486
Cp8 –H12A	3.350	Hp1B –H6A	2.976
Cp8 –H7A	3.459	Hp1B –H10A	2.940
Cp9 –H12C	3.254	Hp1C –H15B	3.394
Cp9 –H9C	3.445	Hp1C –H16A	3.040
Cp9 –H10B	3.053	Hp1C –H16B	2.693
Cp10 –H13B	3.436	Hp2A –H18A	3.184
Cp10 –H14A	3.246	Hp2B –H6B	2.764
Cp10 –Hp5B	3.454	Hp2B –H11A	2.893
C1 –H11B	3.399	Hp2B –H3	3.099
C1 –H12A	3.305	Hp2B –H18A	3.086
C1 –H15B	3.426	Hp2C –H7C	3.456
C2 –H6A	3.466	Hp2C –H16A	2.977
C2 –H11B	2.808	Hp2C –H17A	3.354
C2 –H12A	3.345	Hp3B –H7A	3.262
C3 –H11B	3.399	Hp3B –H7C	3.356
C3 –H12A	3.457	Hp3C –H11A	3.322
C4 –Hp3C	3.395	Hp3C –H12A	2.479
B –H12A	3.263	Hp3C –H12C	3.088
C6 –H2	3.245	Hp3C –H4	3.413
C6 –H3	3.355	Hp3C –H7A	2.844
C9 –H7A	3.468	Hp3C –H7C	3.471
C9 –H9A	3.453	Hp4A –H10B	3.126

Table 5. (Cont.)

	Distance(Å)		Distance(Å)
Hp4B –H12C	2.888	H7B –H17A	3.220
Hp4B –H13B	3.299	H7B –H18C	3.465
Hp4B –H9C	3.409	H7B –H9A	3.189
Hp4B –H10B	2.617	H7B –H9B	3.435
Hp4B –Hp5B	3.377	H7B –H9C	3.351
Hp4C –H12C	3.110	H7C –H16A	3.384
Hp4C –H9C	2.688	H7C –H16B	3.392
Hp4C –H10B	2.981	H7C –H16C	3.470
Hp5A –H13A	3.450	H9A –H12A	3.267
Hp5A –H14A	2.862	H9A –H12B	3.332
Hp5A –H6A	3.395	H9A –H9A	2.736
Hp5A –H6C	3.350	H9A –H9C	3.320
Hp5A –H10A	2.842	H9B –H15A	3.173
Hp5A –H10B	3.033	H9B –H15B	3.189
Hp5B –H13A	3.414	H9B –H16A	3.287
Hp5B –H13B	2.887	H9B –H16C	3.091
Hp5B –H14A	2.891	H9C –H16C	3.275
Hp5B –Hp5B	2.596	H10B –H14A	3.230
Hp5C –H6C	3.344	H10B –H17B	3.228
H1 –H15B	3.003	H10C –H17B	3.026
H1 –H16A	3.055	H14B –H18B	2.952
H2 –H6A	2.689	H14C –H18A	3.259
H2 –H6B	3.187	H14C –H18B	3.230
H2 –H6C	3.403	H15A –H16A	3.007
H2 –H11B	2.595	H15A –H16C	3.103
H3 –H6A	3.497	H16A –H16C	3.255
H3 –H6B	2.927	H16A –H17A	3.343
H3 –H6C	3.161		
H3 –H18A	2.863		
H6C –H18A	3.293		
H6C –H18C	2.953		
H7A –H12A	3.308		
H7A –H9A	3.288		
H7A –H9C	2.931		
H7B –H15A	3.311		

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X-ray I.D. AFK3

Name of Compound Pentamethylcyclopentadienyl Diisopropylamino-borolide Hafnium Chloride · Hydrogen chloride

Chemical Formula $C_{16}H_{32}BCl_2HfN$ M. wt. 498.65

Crystal System Monoclinic Space Group $P2_1/n$ (# 14)

a=	12.073(3)	Å	α=	90°	
b=	15.295(4)	Å	β=	95.58(2)°	
c=	12.314(3)	Å	γ=	90°	
V=	2263.1(10)	Å^3	Z=	4	
D_m	—	g cm^{-3}	D_x	1.46	g cm^{-3}

Radiation used MoKα Wavelength 0.71073 Å

Absorption Coefficient, μ= 48.02 cm^{-1} Temperature 295 °K

Type of Absorption Correction empirical (program used) CRYM

Range of Transmission Factors 0.833 to 1.172, relative.

Crystal Color yellow Crystal Shape (Habit) monoclinic pyramid

Crystal Size .23 mm × .26 mm × .34 mm

Source of Crystal AFK

Type of Diffractometer Enraf-Nonius Cad-4

Data Collection method (diffraction geometry, scan type) θ-2θ scans

Lattice Parameters: Number of reflections 25; θ range 11° to 13°

θ range for data collection 1° to 29°

h_{min} -16 h_{max} 16 k_{min} -20 k_{max} 20 l_{min} 0 l_{max} 16

Number of reflections measured 12875

Number of independent reflections 6012

Number of reflections used in refinement 6012

Criterion for reflections used All used, F_o^2 positive and negative.

Goodness of fit for merging data 1.06 (number of multiples 5798)

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R_{int} for duplicate reflections 0.050 (number of duplicates 4334)

Number of standard reflections 3 Interval 150 min

Variations of standards 0.89% decay during data collection, linear.

How structure solved? Hf atom coordinates found from Patterson map, remaining atoms located by structure factor - Fourier calculations.

How H atoms treated? Cp^*: positioned at idealized locations in difference maps calculated in their expected planes; not repositioned. Remainder: by calculation (C-H, NH = 0.95Å) with staggered geometry, repositioned once. Assigned B = 1.1 x B_{eq} of bonded atom.

Refinement on F^2, $w=1/\sigma^2(F_o^2)$, one full matrix used.

R = 0.071 on F for 5363 reflections with $F_o^2 > 0$

R = 0.037 on F for 3522 reflections with $F_o^2 > 3\sigma(F_o^2)$

wR = 0.005 on F^2 for 6012 reflections

Goodness of Fit (S) = 1.15 for 6012 data and 226 parameters

$(\Delta/\sigma)_{max}$ in final least squares cycle < 0.005

$\Delta\rho_{max}$ +1.96 eÅ^{-3}, $\Delta\rho_{min}$ -1.26 eÅ^{-3} in final difference map. all major peaks near Hf and Cl atoms.

Secondary Extinction parameter (if used) N.A.

(Reference: Larson, A. C. (1967). *Acta Cryst.* **23**, 644-665.)

Computer Programs

The CRYM Crystallographic Computing System

(Duchamp, D. J. (1964). Am. Crystallogr. Assoc. Meet., Bozeman, Montana, Paper B14, p. 29.)

ORTEP

(Johnson, C. K. (1976). *ORTEP*II. Report ORNL-3794. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.)

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MULTAN88

Debaerdemaeker, T., Germain, G., Main, P., Refaat, L. S., Tate, C. & Woolfson, M. M. (1988). *MULTAN 88. Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*, Univs. of York, England and Louvain, Belgium.

Scattering Factors and f', f'':

Cromer, D. T. (1974). *International Tables For X-ray Crystallography*, Vol. IV, pp. 149–151. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Cromer, D. T. & Waber, J. T. (1974). *International Tables For X-ray Crystallography*, Vol. IV, pp. 99–101. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Any additional Data: H atom on N positioned by calculation. A 3-D difference map calculated with final parameters, leaving out HN, showed a wide region of positive (+0.4-0.6 e Å^{-3}) electron density near the calculated position and spreading toward a position between N and Cl 2. The peak of that density, 0.62 e Å^{-3}, was only 0.67 Å from N, so I assumed the calculated position of HN was more likely the better.

Weights w are calculated as $1/\sigma^2(F_o^2)$; variances ($\sigma^2(F_o^2)$) were derived from counting statistics plus an additional term, $(0.014I)^2$; variances of the merged data were obtained by propagation of error plus another additional term, $(0.014\bar{I})^2$.

Definitions:

$$R = \frac{\Sigma||F_o| - |F_c||}{\Sigma F_o}; \quad R_w = \frac{\Sigma w(F_o^2 - F_c^2)}{\Sigma w F_o^2}$$

$$S = \left\{\frac{\Sigma w(F_o^2 - F_c^2)^2}{n-p}\right\}^{\frac{1}{2}}$$

where n = number of data,

p = number of parameters refined.

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Table 1. Final Heavy Atom Parameters for Cp*, Diisopropylaminoborollide Hafnium Chloride · HCl.

x, y, z and $U_{eq}{}^{a} \times 10^4$

Atom	x	y	z	U_{eq}
Hf	2447(.2)	2304(.1)	726(.2)	360(.5)
Cl1	4110(2)	2053(2)	1960(2)	974(7)
Cl2	1859(2)	765(1)	716(1)	786(6)
Cp1	1682(5)	3688(3)	1448(5)	395(13)
Cp2	771(5)	3260(3)	848(5)	421(14)
Cp3	542(5)	2486(3)	1400(5)	477(16)
Cp4	1300(5)	2424(4)	2341(5)	457(14)
Cp5	1991(5)	3167(4)	2378(5)	444(14)
Me1	2117(6)	4592(4)	1261(6)	634(19)
Me2	58(5)	3642(4)	−90(6)	645(19)
Me3	−414(6)	1889(4)	1127(7)	866(25)
Me4	1335(7)	1720(5)	3206(6)	803(22)
Me5	2803(6)	3423(5)	3333(6)	814(23)
C1	1982(5)	2474(3)	−1262(4)	477(15)
C2	2570(7)	3229(4)	−845(5)	586(18)
C3	3651(6)	3022(5)	−459(6)	649(18)
C4	3864(5)	2124(4)	−636(5)	550(17)
B	2843(6)	1756(4)	−1219(5)	418(16)
N	2624(4)	774(3)	−1578(4)	424(11)
C5	1993(7)	626(4)	−2681(6)	753(22)

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Table 1. (Cont.)

Atom	x	y	z	U_{eq}
C6	2261(8)	1288(6)	−3533(6)	1017(32)
C7	766(7)	590(5)	−2577(7)	1030(29)
C8	3649(5)	195(4)	−1345(5)	539(16)
C9	4519(6)	346(5)	−2134(7)	834(23)
C10	3336(6)	−745(4)	−1234(6)	677(19)

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

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Table 2. Assigned Hydrogen Atom Parameters for Cp*, Diisopropylaminoborollide Hafnium Chloride · HCl.

x, y and $z \times 10^4$

Atom	x	y	z	B
HC1A	2013	4745	489	5.7
HC1B	2889	4630	1494	5.7
HC1C	1722	5021	1647	5.7
HC1D	1534	4961	899	5.7
HC1E	2714	4574	797	5.7
HC1F	2376	4861	1934	5.7
HC2A	−611	3901	139	5.7
HC2B	−163	3214	−645	5.7
HC2C	449	4106	−446	5.7
HC2D	−54	4267	10	5.7
HC2E	−665	3375	−189	5.7
HC2F	394	3580	−774	5.7
HC3A	−1086	2102	1426	7.5
HC3B	−278	1307	1418	7.5
HC3C	−601	1830	347	7.5
HC3D	−793	1749	1769	7.5
HC3E	−197	1342	821	7.5
HC3F	−974	2150	602	7.5
HC4A	2091	1523	3394	7.3
HC4B	896	1228	2952	7.3
HC4C	1057	1936	3863	7.3
HC4D	1684	1935	3895	7.3
HC4E	1759	1226	2997	7.3
HC4F	600	1527	3316	7.3
HC5A	3407	3763	3081	7.1
HC5B	3125	2910	3691	7.1
HC5C	2449	3762	3844	7.1
H1	1215	2431	−1513	4.2
H2	2262	3802	−832	5.2
H3	4181	3421	−119	5.7
H4	4534	1815	−422	4.8

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Table 2. (Cont.)

Atom	x	y	z	B
HN	2097	582	−1104	5.0
H5	2232	79	−2934	6.7
H6A	3040	1299	−3580	8.9
H6B	1889	1128	−4220	8.9
H6C	2016	1851	−3333	8.9
H7A	622	170	−2039	9.1
H7B	511	1146	−2372	9.1
H7C	384	423	−3259	9.1
H8	3998	368	−653	4.8
H9A	4681	952	−2166	7.4
H9B	5182	37	−1883	7.4
H9C	4251	141	−2835	7.4
H10A	2792	−793	−729	6.0
H10B	3050	−965	−1921	6.0
H10C	3981	−1069	−969	6.0

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Table 3. Anisotropic Displacement Parameters for Cp*, Diisopropylaminoborollide Hafnium Chloride · HCl.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Hf	433(1)	323(1)	323(1)	69(1)	28(1)	−3(1)
Cl1	705(13)	1506(21)	661(12)	607(13)	−188(10)	−224(12)
Cl2	1491(19)	311(8)	639(11)	−13(9)	526(12)	9(8)
Cp1	422(35)	313(28)	452(33)	67(24)	46(28)	−45(24)
Cp2	396(34)	435(33)	430(32)	162(25)	30(27)	10(26)
Cp3	417(33)	351(38)	670(39)	60(22)	93(30)	10(25)
Cp4	573(37)	381(34)	437(31)	129(27)	155(28)	62(25)
Cp5	440(36)	483(35)	399(33)	171(28)	−7(28)	−137(28)
Me1	733(50)	415(36)	778(49)	−52(32)	195(41)	−51(34)
Me2	514(43)	679(44)	716(47)	172(33)	−76(37)	103(36)
Me3	585(47)	564(43)	1425(78)	−120(36)	−31(50)	129(48)
Me4	1100(65)	757(50)	611(46)	270(44)	378(45)	307(38)
Me5	885(60)	901(56)	602(46)	216(43)	−196(43)	−341(40)
C1	593(38)	502(43)	334(28)	106(27)	33(27)	61(24)
C2	953(53)	389(33)	455(38)	55(39)	268(37)	105(31)
C3	670(48)	585(41)	716(48)	−260(36)	192(41)	−76(36)
C4	477(38)	483(44)	722(44)	−27(28)	216(34)	−41(31)
B	595(47)	385(36)	295(32)	13(31)	156(32)	26(27)
N	472(30)	437(27)	382(26)	31(22)	140(23)	−27(21)
C5	1021(68)	589(45)	609(46)	57(42)	−117(46)	−201(36)
C6	1598(94)	1111(68)	338(38)	168(60)	80(50)	117(41)
C7	875(68)	952(64)	1162(74)	−111(50)	−414(59)	23(55)
C8	633(44)	426(34)	576(40)	67(30)	144(35)	−26(29)
C9	777(56)	693(49)	1099(65)	129(39)	438(51)	−139(45)
C10	783(54)	541(41)	723(48)	127(35)	155(42)	−35(36)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*^2} + U_{22}k^2b^{*^2} + U_{33}\ell^2c^{*^2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

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Table 4. Complete Distances and Angles for Cp*, Diisopropylaminoborollide Hafnium Chloride · HCl.

	Distance(Å)		Distance(Å)
Hf –Cl1	2.428(2)	Me2 –HC2D	0.974
Hf –Cl2	2.458(2)	Me2 –HC2E	0.960
Hf –Cp*	2.221	Me2 –HC2F	0.974
Hf –CpB	2.169	Me3 –HC3A	0.979
Cp1 –Cp2	1.424(8)	Me3 –HC3B	0.967
Cp1 –Cp5	1.415(8)	Me3 –HC3C	0.969
Cp1 –Me1	1.505(8)	Me3 –HC3D	0.975
Cp2 –Cp3	1.406(8)	Me3 –HC3E	0.965
Cp2 –Me2	1.491(8)	Me3 –HC3F	0.975
Cp3 –Cp4	1.409(8)	Me4 –HC4A	0.967
Cp3 –Me3	1.484(9)	Me4 –HC4B	0.956
Cp4 –Cp5	1.408(8)	Me4 –HC4C	0.963
Cp4 –Me4	1.513(9)	Me4 –HC4D	0.968
Cp5 –Me5	1.507(9)	Me4 –HC4E	0.962
C1 –C2	1.424(9)	Me4 –HC4F	0.957
C1 –B	1.509(8)	Me5 –HC5A	0.971
C2 –C3	1.381(10)	Me5 –HC5B	0.963
C3 –C4	1.418(9)	Me5 –HC5C	0.948
C4 –B	1.476(9)	C1 –H1	0.950
B –N	1.580(8)	C2 –H2	0.953
N –C5	1.509(9)	C3 –H3	0.951
N –C8	1.526(8)	C4 –H4	0.951
C5 –C6	1.515(11)	N –HN	0.951
C5 –C7	1.500(11)	C5 –H5	0.948
C8 –C9	1.516(10)	C6 –H6A	0.947
C8 –C10	1.496(9)	C6 –H6B	0.951
Me1 –HC1A	0.975	C6 –H6C	0.950
Me1 –HC1B	0.950	C7 –H7A	0.951
Me1 –HC1C	0.963	C7 –H7B	0.948
Me1 –HC1D	0.975	C7 –H7C	0.953
Me1 –HC1E	0.962	C8 –H8	0.951
Me1 –HC1F	0.951	C9 –H9A	0.950
Me2 –HC2A	0.965	C9 –H9B	0.954
Me2 –HC2B	0.965	C9 –H9C	0.946
Me2 –HC2C	0.979	C10 –H10A	0.949

Table 4. (Cont.)

Distance(Å)		Angle(°)			
C10 –H10B	0.945	Cl1	–Hf	–Cl2	94.1(1)
C10 –H10C	0.953	Cp*	–Hf	–CpB	132.6
		Cp*	–Hf	–Cl1	106.4
		Cp*	–Hf	–Cl2	105.3
		CpB	–Hf	–Cl1	107.1
		CpB	–Hf	–Cl2	104.7
		Cp5	–Cp1	–Cp2	106.9(5)
		Me1	–Cp1	–Cp2	127.3(5)
		Me1	–Cp1	–Cp5	124.9(5)
		Cp3	–Cp2	–Cp1	108.3(5)
		Me2	–Cp2	–Cp1	125.5(5)
		Me2	–Cp2	–Cp3	125.3(5)
		Cp4	–Cp3	–Cp2	108.2(5)
		Me3	–Cp3	–Cp2	126.4(5)
		Me3	–Cp3	–Cp4	125.0(5)
		Cp5	–Cp4	–Cp3	107.9(5)
		Me4	–Cp4	–Cp3	126.8(5)
		Me4	–Cp4	–Cp5	125.2(5)
		Cp4	–Cp5	–Cp1	108.6(5)
		Me5	–Cp5	–Cp1	125.8(5)
		Me5	–Cp5	–Cp4	125.0(5)
		B	–C1	–C2	105.1(5)
		C3	–C2	–C1	111.1(6)
		C4	–C3	–C2	110.4(6)
		B	–C4	–C3	106.8(5)
		C4	–B	–C1	106.2(5)
		N	–B	–C1	125.9(5)
		N	–B	–C4	127.3(5)
		C5	–N	–B	116.7(5)
		C8	–N	–B	112.9(4)
		C8	–N	–C5	114.3(5)
		C6	–C5	–N	113.5(6)
		C7	–C5	–N	110.2(6)
		C7	–C5	–C6	111.3(6)
		C9	–C8	–N	113.0(5)

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Table 4. (Cont.)

	Angle(°)		Angle(°)
C10 –C8 –N	111.6(5)	HC3E –Me3 –HC3D	106.9
C10 –C8 –C9	113.7(5)	HC3F –Me3 –HC3D	106.1
HC1A –Me1 –Cp1	110.8	HC3F –Me3 –HC3E	107.0
HC1B –Me1 –Cp1	110.9	HC4A –Me4 –Cp4	110.5
HC1C –Me1 –Cp1	110.6	HC4B –Me4 –Cp4	110.7
HC1D –Me1 –Cp1	110.7	HC4C –Me4 –Cp4	110.9
HC1E –Me1 –Cp1	110.9	HC4D –Me4 –Cp4	110.8
HC1F –Me1 –Cp1	110.8	HC4E –Me4 –Cp4	110.5
HC1B –Me1 –HC1A	108.1	HC4F –Me4 –Cp4	110.9
HC1C –Me1 –HC1A	107.1	HC4B –Me4 –HC4A	108.3
HC1C –Me1 –HC1B	109.2	HC4C –Me4 –HC4A	107.7
HC1E –Me1 –HC1D	107.1	HC4C –Me4 –HC4B	108.6
HC1F –Me1 –HC1D	108.0	HC4E –Me4 –HC4D	107.7
HC1F –Me1 –HC1E	109.2	HC4F –Me4 –HC4D	108.2
HC2A –Me2 –Cp2	111.8	HC4F –Me4 –HC4E	108.7
HC2B –Me2 –Cp2	112.5	HC5A –Me5 –Cp5	109.9
HC2C –Me2 –Cp2	111.3	HC5B –Me5 –Cp5	110.4
HC2D –Me2 –Cp2	111.2	HC5C –Me5 –Cp5	111.0
HC2E –Me2 –Cp2	112.4	HC5B –Me5 –HC5A	107.4
HC2F –Me2 –Cp2	111.9	HC5C –Me5 –HC5A	108.6
HC2B –Me2 –HC2A	107.8	HC5C –Me5 –HC5B	109.3
HC2C –Me2 –HC2A	106.6	H1 –C1 –C2	127.6
HC2C –Me2 –HC2B	106.6	H1 –C1 –B	127.4
HC2E –Me2 –HC2D	107.3	H2 –C2 –C1	124.7
HC2F –Me2 –HC2D	106.2	H2 –C2 –C3	124.2
HC2F –Me2 –HC2E	107.4	H3 –C3 –C2	125.3
HC3A –Me3 –Cp3	111.4	H3 –C3 –C4	124.3
HC3B –Me3 –Cp3	112.5	H4 –C4 –C3	126.8
HC3C –Me3 –Cp3	112.5	H4 –C4 –B	126.4
HC3D –Me3 –Cp3	111.6	HN –N –B	103.1
HC3E –Me3 –Cp3	112.9	HN –N –C5	101.3
HC3F –Me3 –Cp3	111.9	HN –N –C8	106.5
HC3B –Me3 –HC3A	106.5	H5 –C5 –N	106.5
HC3C –Me3 –HC3A	106.3	H5 –C5 –C6	105.7
HC3C –Me3 –HC3B	107.2	H5 –C5 –C7	109.3

Table 4. (Cont.)

			Angle(°)
H6A	–C6	–C5	109.5
H6B	–C6	–C5	109.2
H6C	–C6	–C5	109.4
H6B	–C6	–H6A	109.6
H6C	–C6	–H6A	109.7
H6C	–C6	–H6B	109.3
H7A	–C7	–C5	109.5
H7B	–C7	–C5	109.8
H7C	–C7	–C5	109.3
H7B	–C7	–H7A	109.6
H7C	–C7	–H7A	109.2
H7C	–C7	–H7B	109.4
H8	–C8	–N	106.7
H8	–C8	–C9	104.9
H8	–C8	–C10	106.2
H9A	–C9	–C8	109.4
H9B	–C9	–C8	109.2
H9C	–C9	–C8	109.7
H9B	–C9	–H9A	109.2
H9C	–C9	–H9A	109.9
H9C	–C9	–H9B	109.5
H10A	–C10	–C8	109.4
H10B	–C10	–C8	109.5
H10C	–C10	–C8	109.0
H10B	–C10	–H10A	110.0
H10C	–C10	–H10A	109.2
H10C	–C10	–H10B	109.6

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Table 5. Intermolecular Distances Less than 3.5Åfor Cp*, Diisopropylaminoborollide Hafnium Chloride · HCl.

	Distance(Å)		Distance(Å)
Cl1 –HC2B	3.022	Me5 –H10A	3.328
Cl1 –HC2F	3.208	C1 –H10B	3.270
Cl1 –H1	3.112	C2 –H5	3.225
Cl1 –H7B	3.295	C2 –H10B	3.042
Cl1 –H9B	3.313	C3 –HC4C	3.101
Cl1 –H10C	3.102	C3 –HC4F	2.997
Cl2 –HC1F	3.259	C4 –HC4C	3.127
Cl2 –HC5A	3.431	C4 –HC4F	3.294
Cl2 –HC5C	3.208	C6 –HC4D	3.327
Cp1 –H9A	3.139	C6 –HC2A	3.190
Cp1 –H9B	3.469	C6 –HC2E	3.418
Cp2 –H9A	3.129	C6 –HC3A	3.172
Cp3 –H9A	3.204	C6 –HC3F	3.438
Cp4 –H9A	3.253	C7 –HC5A	3.194
Cp5 –H9A	3.196	C7 –HC3B	3.311
Me1 –H9B	3.471	C7 –HC4B	3.432
Me1 –HC4A	3.121	C9 –HC1C	3.227
Me1 –HC4E	2.946	C10 –HC5C	3.266
Me1 –HC2A	3.314	C10 –HC3A	3.409
Me1 –HC2D	3.308	C10 –HC3D	3.438
Me2 –H6A	3.207	HC1A –H5	3.398
Me2 –HC1C	3.416	HC1A –H6A	3.339
Me2 –HC1D	2.980	HC1A –H6B	3.013
Me2 –HC2D	3.200	HC1A –HC4A	3.190
Me3 –H6A	3.381	HC1A –HC4E	3.204
Me3 –HC5B	3.343	HC1A –HC2A	2.738
Me3 –H7A	3.361	HC1A –HC2C	3.448
Me3 –H10A	3.320	HC1A –HC2D	2.824
Me4 –H6B	3.301	HC1A –HC2E	3.307
Me4 –H3	3.479	HC1B –H7C	2.999
Me4 –HC1B	3.340	HC1B –HC4A	2.899
Me4 –HC1C	3.494	HC1B –HC4B	2.897
Me4 –HC1F	3.253	HC1B –HC4E	2.545
Me5 –HC3C	3.014	HC1B –HC4F	3.422
Me5 –HC3F	3.154	HC1C –H9A	3.336

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Table 5. (Cont.)

	Distance(Å)		Distance(Å)
HC1C –H9B	2.720	HC2A –HC2C	3.075
HC1C –H9C	3.121	HC2A –HC2D	2.926
HC1C –HC4A	2.712	HC2B –HC4A	3.434
HC1C –HC4B	3.413	HC2B –HC5B	2.752
HC1C –HC4E	2.607	HC2C –H9C	2.696
HC1C –HC2A	2.963	HC2C –HC2C	3.177
HC1C –HC2B	3.450	HC2C –HC2D	2.600
HC1C –HC2C	3.175	HC2D –H6A	3.136
HC1C –HC2D	2.933	HC2D –H9C	3.000
HC1C –HC2E	3.229	HC2D –H9C	3.226
HC1C –HC2F	3.424	HC2D –HC2D	2.248
HC1D –H9B	3.315	HC2D –HC2F	3.460
HC1D –H9C	3.299	HC2E –H6A	2.688
HC1D –H6B	3.443	HC2E –H6B	3.377
HC1D –HC4A	2.991	HC2E –HC4A	3.081
HC1D –HC4E	3.049	HC2E –HC4D	3.322
HC1D –HC2A	2.373	HC2E –HC5B	2.740
HC1D –HC2B	3.245	HC2F –H9C	2.993
HC1D –HC2C	2.796	HC3A –H6A	2.664
HC1D –HC2D	2.335	HC3A –H6C	2.836
HC1D –HC2E	2.858	HC3A –HC5B	3.410
HC1D –HC2F	3.218	HC3A –H10A	2.941
HC1E –H7C	3.319	HC3A –H10B	3.049
HC1E –H6B	3.135	HC3B –H7A	2.433
HC1E –HC4A	3.145	HC3B –H7C	3.496
HC1E –HC4B	3.330	HC3B –H10A	3.170
HC1E –HC4E	2.968	HC3C –HC5A	3.065
HC1F –HC4A	2.663	HC3C –HC5B	2.464
HC1F –HC4B	2.947	HC3C –HC5C	2.990
HC1F –HC4E	2.331	HC3C –H10A	3.158
HC2A –H6A	2.396	HC3D –H6A	3.313
HC2A –H6B	3.194	HC3D –H6C	3.397
HC2A –H9A	3.311	HC3D –H7A	2.957
HC2A –H9C	2.913	HC3D –H10A	3.000
HC2A –HC4A	3.403	HC3D –H10B	2.999

Table 5. (Cont.)

	Distance(Å)		Distance(Å)
HC3E –HC5B	3.355	H2 –H5	2.585
HC3E –H7A	2.829	H2 –H9C	3.105
HC3E –H10A	3.234	H2 –H10B	2.780
HC3F –H6A	2.881	H3 –H6B	3.418
HC3F –H6C	3.251	H3 –H7C	3.136
HC3F –HC5A	3.419	H4 –H10C	2.618
HC3F –HC5B	2.496	H6C –H10B	3.357
HC3F –HC5C	3.074	H6C –H10C	3.480
HC3F –H10A	3.035	H8 –H8	2.992
HC4A –H6B	3.032	H8 –H9B	3.242
HC4B –H3	3.342	H8 –H10C	3.185
HC4B –H7A	2.964		
HC4B –H7C	3.003		
HC4C –H6B	2.766		
HC4C –H3	2.748		
HC4C –H4	2.849		
HC4D –H6B	2.619		
HC4D –H6C	3.400		
HC4D –H3	3.408		
HC4D –H4	3.395		
HC4E –H6B	3.418		
HC4F –H6B	3.328		
HC4F –H3	2.701		
HC4F –H4	3.301		
HC4F –H7A	3.306		
HC4F –H7C	3.209		
HC5A –H7A	3.149		
HC5A –H7B	2.657		
HC5A –H7C	3.277		
HC5B –H10A	3.464		
HC5C –H9A	3.478		
HC5C –H9B	3.345		
HC5C –H10A	2.464		
HC5C –H10C	3.282		
H1 –H10B	3.295		

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Table 6. Observed and Calculated Structure Factors for Zirconium Cp*, C_4B-Ring Chloride, LiCl Dietherate.

The columns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\sigma F_{obs}$. A minus sign preceding F_{obs} indicates that F^2_{obs} is negative.

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-11 0 l

1	153	159	23
3	362	366	13
5	56	20	48
7	125	117	28

-11 1 l

1	30	50	48
2	105	97	23
3	145	100	17
4	87	94	27
5	286	246	10
6	-54	15	35
7	55	32	35

-11 2 l

1	113	99	21
2	58	45	34
3	147	155	18
4	173	175	15
5	91	95	25
6	150	126	17
7	146	83	16

-11 3 l

1	44	57	41
2	165	153	16
3	148	102	17
4	57	66	35
5	-9	27	63
6	140	145	19

-11 4 l

1	55	31	35
2	40	19	41
3	-48	15	38
4	249	226	11
5	98	79	24
6	57	36	34

-11 5 l

1	50	59	38
2	23	103	54
3	85	6	25
4	78	41	28
5	-45	32	40
6	189	194	14

-11 6 l

1	38	10	43
2	101	4	22
3	64	13	32
4	218	173	12
5	153	120	16

-11 7 l

1	31	28	47
2	124	131	20
3	32	99	48
4	46	76	40

-11 8 l

1	43	67	42
2	-72	17	29
3	21	96	55

-10 0 l

2	158	135	21
4	552	551	11
6	135	154	24
8	23	26	63

-10 1 l

1	-31	54	46
2	427	450	8
3	133	128	18
4	63	60	32
5	113	127	20
6	225	198	11
7	76	104	27
8	154	166	16
9	-37	7	43

-10 2 l

1	195	219	13
2	-64	47	31
3	245	253	11
4	327	321	9
5	127	60	18
6	-31	14	45
7	120	101	19
8	-9	23	62
9	171	166	15

-10 3 l

1	34	73	44
2	56	79	34
3	270	265	10
4	45	81	38
5	176	195	14
6	101	95	22
7	12	42	58
8	44	60	39
9	63	76	33

-10 4 l

1	129	117	18
2	88	48	24
3	135	164	17
4	48	2	37
5	301	310	10
6	-30	76	46
7	193	164	12
8	63	38	32
9	174	185	16

-10 5 l

1	-71	29	28
2	-52	7	35
3	259	260	10
4	-97	28	23
5	128	100	18
6	-71	46	29
7	56	87	46
8	-14	14	58

-10 6 l

1	148	162	16
2	103	76	21
3	65	91	31
4	18	51	55
5	247	276	11
6	-48	19	37
7	177	153	20
8	28	55	49

-10 7 l

1	48	3	37
2	14	37	58
3	283	276	10
4	150	49	15
5	109	119	21
7	79	4	36
8	73	91	30

-10 8 l

1	233	238	12
2	-71	18	29
3	143	158	18
4	117	166	21
7	83	68	36

-10 9 l

1	-33	12	46
2	242	236	12
3	166	144	15
7	53	4	47

-9 0 l

1	541	528	10
3	209	173	16
5	202	200	16
7	272	278	14
9	332	301	13

-9 1 l

1	58	90	32
2	171	166	13
3	494	487	7
4	90	57	23
5	235	220	10
6	127	105	17
7	149	143	15
8	239	240	11
9	246	231	11

-9 2 l

1	320	323	9
2	213	199	11
3	161	165	14
4	316	314	8
5	216	184	11
6	253	241	10
7	187	173	13
8	-60	29	33
9	160	133	15

-9 3 l

1	106	121	20
2	345	348	8
3	302	285	9
4	88	49	22
5	48	51	35
6	173	217	14
7	83	45	25
8	355	334	8
9	168	165	15

-9 4 l

1	160	163	14
2	94	75	22
3	-79	27	25
4	342	349	8
5	176	150	13
6	-34	9	41
7	130	95	17
8	162	147	15
9	106	2	21

-9 5 l

1	81	30	24
2	284	303	9
3	138	120	16
4	218	194	11
5	32	44	42
6	258	237	10
7	29	67	45
8	142	180	18
9	-50	69	48

-9 6 l

1	-45	0	37
2	242	216	10
3	-102	43	21
4	319	304	9
5	30	19	45
6	58	50	32
7	-53	53	34
8	170	142	14

-9 7 l

1	-25	47	49
2	266	299	10
3	189	127	12
4	250	226	10
5	75	50	26
6	249	234	10
7	-89	12	24
8	256	246	11

-9 8 l

1	354	345	8
2	319	305	9
3	112	123	20
4	309	287	9
5	201	142	12
6	90	49	23
7	174	166	14

-9 9 l

1	99	10	23
2	189	172	14
3	414	419	8
4	105	110	22
5	242	254	11
6	79	90	26
7	127	89	18

-9 10 l

1	395	411	8
2	-54	25	35
3	203	205	13
4	-74	0	28
5	178	166	14
6	30	6	46

-9 11 l

1	-83	6	27
2	52	49	36
3	277	301	11
4	115	35	19
5	178	169	14

-9 12 l

1	192	202	13
2	130	130	18
3	94	43	23

-8 0 l

2	610	600	9
4	409	375	10
6	199	233	16
8	298	273	13
10	344	340	12

-8 1 1

1	211	221	11
2	209	235	11
3	180	177	12
4	71	83	26
5	74	46	24
6	335	299	8
7	54	50	32
8	426	428	8
9	227	200	11
10	55	53	34
11	71	82	28

-8 2 1

1	251	295	9
2	382	352	7
3	220	175	10
4	248	246	9
5	305	276	8
6	250	230	9
7	382	375	8
8	249	241	10
9	61	70	32
10	156	171	15
11	67	70	29

-8 3 1

1	160	172	14
2	287	297	8
3	341	318	8
4	51	98	33
5	161	176	13
6	58	73	29
7	109	114	19
8	117	114	19
9	335	359	9
10	169	157	14

-8 4 1

1	473	466	7
2	154	153	14
3	86	93	22
4	148	124	14
5	139	111	15
6	53	10	32
7	318	324	8
8	127	149	17
9	-48	64	35
10	69	70	29

-8 5 1

1	-43	12	36
2	-55	27	31
3	283	280	9
4	96	148	21
5	283	270	9
6	121	69	16
7	-71	17	26
8	33	44	42
9	332	343	9
10	40	23	40

-8 6 1

1	462	436	7
2	123	98	17
3	158	125	13
4	49	16	33
5	63	106	29
6	137	124	15
7	348	355	8
8	70	49	27
9	73	60	27
10	-22	79	51

-8 7 1

1	161	156	14
2	83	121	24
3	320	324	8
4	151	116	14
5	220	207	11
6	-43	20	36
7	7	18	60
8	56	45	32
9	389	361	8

-8 8 1

1	239	251	10
2	354	375	8
3	167	170	14
4	231	236	10
5	168	159	13
6	139	152	16
7	400	389	8
8	132	128	18
9	106	120	21

-8 9 1

1	120	112	18
2	273	277	10
3	207	182	12
4	240	223	10
5	47	62	36
6	313	311	9
7	32	4	45
8	324	302	9
9	190	166	13

-8 10 1

1	-37	19	42
2	599	585	8
3	43	12	38
4	372	368	8
5	-73	29	27
6	206	179	12
7	-59	1	32
8	224	182	12

-8 11 1

1	65	77	30
2	318	304	9
3	96	83	22
4	187	163	13
5	48	66	35
6	222	195	11
7	56	27	32

-8 12 1

1	9	108	63
2	275	268	10
3	52	47	35
4	161	153	15
5	148	106	15
6	119	106	19
7	234	213	12

-8 13 1

1	-79	78	27
2	117	161	19
3	145	110	16
4	-88	31	24
5	-76	76	27
6	-95	55	23

-8 14 1

1	217	237	13
2	84	71	25
3	-23	6	49
4	84	21	24

-7 0 1

1	288	264	11
3	279	333	11
5	316	345	10
7	549	547	9
9	57	24	42
11	241	256	15

-7 1 1

1	668	665	7
2	281	321	8
3	353	353	7
4	197	234	10
5	310	297	7
6	84	160	22
7	265	283	9
8	186	168	12
9	574	574	7
10	80	91	25
11	228	228	11
12	83	98	26

-7 2 1

1	582	587	7
2	392	417	7
3	116	142	15
4	131	129	14
5	-68	59	25
6	-23	22	45
7	402	388	7
8	328	340	8
9	57	89	32
10	213	229	11
11	148	116	15
12	136	114	17

-7 3 1

1	133	166	14
2	371	389	7
3	150	128	12
4	72	68	23
5	474	476	7
6	305	314	8
7	175	116	12
8	167	164	13
9	151	163	14
10	154	184	15
11	-1	30	67
12	128	143	18

-7 4 1

1	337	337	7
2	464	440	7
3	292	282	7
4	30	44	39
5	141	187	14
6	124	131	16
7	106	57	18
8	391	385	8
9	130	126	16
10	126	129	17
11	47	27	36

-7 5 1

1	90	6	20
2	214	221	10
3	71	10	23
4	54	114	30
5	80	63	22
6	360	349	7
7	68	62	26
8	137	127	15
9	33	36	42
10	222	202	11
11	54	19	32

-7 6 1

1	307	314	8
2	381	366	7
3	149	154	13
4	329	309	7
5	68	38	25
6	175	167	12
7	146	135	15
8	420	431	8
9	-80	3	24
10	180	187	13
11	13	1	56

-7 7 1

1	82	41	22
2	44	37	34
3	246	273	9
4	61	52	28
5	310	305	8
6	489	490	7
7	83	3	23
8	226	222	10
9	49	34	34
10	166	175	15
11	-58	56	32

-7 8 1

1	394	398	7
2	236	235	10
3	61	12	28
4	183	169	11
5	249	225	9
6	126	115	17
7	328	352	9
8	379	398	8
9	68	55	29
10	167	224	15

-7 9 1

1	500	493	7
2	215	183	10
3	351	325	8
4	75	12	24
5	297	321	9
6	263	249	9
7	201	195	12
8	96	111	22
9	278	275	9
10	92	49	23

-7 10 1

1	271	238	9
2	-12	19	55
3	299	264	8
4	-31	36	42

5	367	348	8
6	94	62	21
7	469	473	8
8	80	8	25
9	-42	35	39

-7 11 l

1	463	465	7
2	128	36	16
3	245	266	10
4	78	70	25
5	215	238	11
6	218	239	11
7	140	130	16
8	64	82	30
9	216	214	12

-7 12 l

1	279	293	9
2	166	139	13
3	88	76	22
4	161	146	14
5	96	99	21
6	-31	54	44
7	233	211	11
8	225	234	11

-7 13 l

1	149	147	16
2	47	92	36
3	175	175	13
4	-86	4	24
5	121	126	18
6	244	238	10
7	66	9	29
8	124	129	19

-7 14 l

1	198	195	12
2	221	216	11
3	-100	1	21
4	103	123	21
5	-74	9	27
6	64	65	30
7	42	53	40

-7 15 l

1	-63	4	31
2	76	77	26
3	67	30	28
4	74	37	27
5	112	35	19

-7 16 l

1	131	156	18
2	268	255	10
3	-24	49	49
4	103	39	21

-6 0 l

2	926	838	10
4	217	245	11
6	355	344	9
8	714	677	10
10	378	382	11
12	13	95	70

-6 1 l

1	168	160	9
2	303	286	6
3	159	144	10
4	346	330	6
5	53	29	26
6	745	724	7
7	479	466	7
8	79	98	23
9	181	169	11
10	262	279	10
11	129	131	17
12	430	425	8

-6 2 l

1	161	137	10
2	509	532	6
3	453	417	6
4	521	528	6
5	616	577	7
6	-18	22	46
7	267	230	8
8	401	431	7
9	194	168	11
10	311	299	8
11	235	235	10
12	-55	63	34

-6 3 l

1	575	586	6
2	32	21	32
3	81	107	18
4	285	298	7
5	289	284	7
6	313	354	7
7	520	495	7
8	45	66	33
9	285	299	8
10	77	54	24
11	220	217	11
12	154	157	16

-6 4 l

1	233	236	8
2	-73	62	19
3	62	51	22
4	176	164	10
5	325	339	7
6	204	199	10
7	359	375	7
8	83	54	22
9	-56	28	30
10	-56	69	31
11	198	200	12
12	-19	37	53

-6 5 l

1	639	637	7
2	59	17	23
3	194	198	9
4	217	200	8
5	419	431	6
6	199	209	10
7	170	170	12
8	91	86	20
9	265	275	9
10	86	21	22
11	169	199	14
12	100	52	21

-6 6 l

1	428	459	6
2	359	378	6
3	152	194	11
4	275	288	8
5	232	259	9
6	135	122	14
7	347	343	7
8	81	114	23
9	-74	35	25
10	39	49	38
11	222	231	11
12	-42	25	39

-6 7 l

1	427	454	6
2	-71	15	22
3	211	192	9
4	96	81	17
5	53	81	29
6	393	418	7
7	403	391	7
8	172	189	13
9	305	285	8
10	-55	21	32
11	164	165	15
12	48	94	37

-6 8 l

1	119	159	15
2	389	391	7
3	317	291	7
4	243	277	9
5	442	431	7
6	48	26	32
7	164	132	13
8	266	279	9
9	180	206	13
10	188	186	13
11	252	223	10

-6 9 l

1	194	200	10
2	245	240	9
3	-67	15	25
4	259	277	9
5	66	20	26
6	577	561	7
7	329	339	8
8	122	89	17
9	129	112	17
10	175	173	14
11	77	97	27

-6 10 l

1	-16	19	49
2	248	237	9
3	22	53	45
4	338	330	8
5	116	111	17
6	165	134	13
7	102	40	20
8	417	408	8
9	-38	45	39
10	247	239	11

-6 11 l

1	88	83	21
2	111	130	18
3	-64	32	27
4	210	187	11
5	-27	52	44
6	584	570	7
7	177	152	13
8	32	2	43
9	134	136	17
10	137	86	16

-6 12 l

1	87	97	22
2	264	274	9
3	81	81	23
4	366	364	8
5	253	253	10
6	74	2	25
7	159	154	14
8	274	242	9
9	111	108	20

-6 13 l

1	241	243	10
2	75	38	25
3	323	304	8
4	27	89	45
5	165	165	14
6	366	339	8
7	286	290	9
8	-21	6	51
9	162	164	15

-6 14 l

1	360	366	8
2	121	116	18
3	-50	18	34
4	197	192	12
5	274	293	9
6	-66	16	30
7	223	228	12
8	61	88	32

-6 15 l

1	325	317	9
2	163	175	14
3	305	298	9
4	-27	50	46
5	173	171	14
6	49	95	36
7	156	169	16

-6 16 l

1	107	95	21
2	119	129	19
3	-56	25	32
4	121	117	18
5	242	224	11
6	110	42	20

-6 17 l

1	248	226	11
2	104	117	21
3	107	73	20
4	-48	36	37
5	56	55	34

-6 18 l

1	120	81	19
2	206	206	12

-5 0 l

1	279	262	8
3	578	635	7
5	732	788	9
7	-24	126	51
9	151	108	17
11	638	652	10
13	316	321	13

-5 1 l

1	964	980	8
2	156	144	8
3	821	849	7
4	225	274	7
5	-56	23	22
6	36	15	30
7	464	495	6
8	256	240	8
9	308	314	8
10	88	105	21
11	222	236	11
12	236	223	11
13	306	314	9

-5 2 l

1	73	66	16
2	477	501	5
3	413	391	5
4	206	194	7
5	818	825	8
6	528	553	6
7	253	238	8
8	125	128	14
9	-32	10	39
10	258	272	9
11	352	373	8
12	-66	64	29
13	201	191	12

-5 3 l

1	741	698	7
2	354	338	5
3	630	632	6
4	749	744	7
5	441	423	6
6	380	411	6
7	300	286	7
8	56	36	27
9	165	142	12
10	156	133	14
11	106	137	20
12	372	369	8
13	140	121	16

-5 4 l

1	151	114	9
2	862	891	8
3	38	68	27
4	739	773	7
5	400	389	6
6	223	204	8
7	176	160	11
8	301	288	7
9	54	57	30
10	485	492	7
11	105	70	20
12	25	22	47
13	96	24	21

-5 5 l

1	82	53	16
2	56	57	21
3	197	207	8
4	730	742	7
5	185	181	9
6	1023	1011	9
7	-23	2	42
8	228	228	9
9	158	125	13
10	137	83	15
11	80	23	24
12	328	354	9
13	64	73	31

-5 6 l

1	159	163	9
2	623	601	6
3	142	99	10
4	709	705	7
5	368	388	6
6	316	322	7
7	316	302	7
8	343	334	7
9	157	143	13
10	377	394	8
11	-29	16	43
12	155	98	15

-5 7 l

1	380	411	6
2	128	119	11
3	237	253	7
4	465	428	6
5	376	351	6
6	468	475	7
7	310	290	8
8	200	195	11
9	180	174	12
10	215	208	11
11	148	127	15
12	387	406	8

-5 8 l

1	29	1	33
2	-33	81	33
3	51	45	25
4	101	72	16
5	509	507	6
6	471	441	7
7	180	191	12
8	132	137	15
9	65	36	27
10	132	125	17
11	351	344	9
12	84	92	26

-5 9 l

1	200	180	9
2	155	165	11
3	259	264	8
4	285	237	7
5	-57	2	27
6	68	25	25
7	449	430	7
8	213	221	11
9	369	381	8
10	88	110	23
11	47	131	39
12	231	220	12

-5 10 l

1	107	99	16
2	53	51	27
3	106	130	17
4	65	83	25
5	502	488	7
6	87	79	21
7	46	99	33
8	85	63	23
9	186	161	12
10	-39	16	39
11	511	520	8

-5 11 l

1	390	388	7
2	80	97	22
3	423	392	7
4	98	79	18
5	-22	42	46
6	121	91	16
7	393	381	8
8	35	30	41
9	348	335	8
10	184	154	13
11	182	198	15

-5 12 l

1	173	153	12
2	78	79	22
3	137	117	14
4	64	40	27
5	609	611	7
6	220	227	10
7	190	172	12
8	234	223	10
9	50	32	34
10	130	157	18

-5 13 l

1	337	341	8
2	78	8	23
3	432	442	7
4	230	216	10
5	206	197	11
6	325	312	8
7	241	228	10
8	-40	6	38
9	105	62	20
10	40	76	41

-5 14 l

1	38	24	38
2	472	442	7
3	-29	20	43
4	432	432	7
5	343	326	8
6	217	188	11
7	93	50	22
8	257	246	10
9	2	8	67

-5 15 l

1	22	41	48
2	177	158	13
3	-98	31	21
4	302	305	9
5	58	10	32
6	413	416	8
7	-61	66	31
8	142	103	16

-5 16 l

1	238	225	10
2	239	236	10
3	-47	21	35
4	360	353	8
5	81	116	26
6	105	161	22
7	136	117	17

-5 17 l

1	227	200	11
2	70	44	28
3	299	297	9
4	145	134	16
5	80	69	26
6	222	219	12

-5 18 l

1	88	78	23
2	77	28	26
3	-70	5	28
4	105	115	21
5	217	215	12

-5 19 l

1	185	179	14
2	-43	33	38

-4 0 l

2	813	817	9
4	696	687	8
6	602	583	8
8	191	180	13
10	288	255	11
12	547	544	10
14	234	203	16

-4 1 l

1	-49	20	21
2	506	534	5
3	249	212	5
4	992	958	9
5	71	4	16
6	367	346	5
7	262	225	7
8	101	84	16
9	77	55	22
10	433	425	7
11	119	66	17
12	315	322	9
13	123	125	18
14	87	66	25

-4 2 l

1	369	386	5
2	1607	1596	14
3	310	328	5
4	451	452	5
5	732	733	7
6	397	419	5
7	71	58	19
8	246	226	8
9	6	62	56
10	339	366	8
11	423	382	7
12	269	262	9
13	-55	10	32

-4 3 l

1	180	130	7
2	185	231	7
3	964	913	8
4	1274	1323	11
5	192	194	7
6	446	479	6
7	402	434	6
8	256	248	8
9	346	360	7
10	61	70	28
11	111	108	19
12	321	306	9
13	236	206	11

-4 4 l

1	650	639	6
2	784	811	7
3	663	676	6
4	448	459	5

5	967	972	9
6	171	171	9
7	479	463	6
8	-45	12	30
9	-32	105	39
10	269	253	9
11	507	521	7
12	-49	14	34
13	119	100	18

-4 5 1

1	708	711	6
2	65	85	17
3	1335	1365	11
4	139	145	9
5	260	268	7
6	75	11	17
7	400	399	6
8	-15	33	47
9	541	552	7
10	-11	41	55
11	200	200	12
12	-49	13	34
13	184	170	13

-4 6 1

1	206	174	6
2	418	403	5
3	781	754	7
4	164	200	9
5	1136	1153	10
6	49	104	27
7	114	84	14
8	76	95	22
9	106	32	17
10	269	267	9
11	520	512	7
12	102	30	20
13	138	113	17

-4 7 1

1	138	128	10
2	164	175	8
3	747	787	7
4	732	768	7
5	489	492	6
6	252	256	7
7	304	299	7
8	130	159	14
9	226	219	10
10	-36	72	39
11	34	10	42
12	290	265	9
13	221	223	12

-4 8 1

1	298	323	6
2	561	583	6
3	225	279	7
4	329	336	6
5	426	424	6
6	350	342	7
7	162	158	11
8	101	117	18
9	127	122	16
10	392	376	8
11	350	343	8
12	170	161	14

-4 9 1

1	81	99	17
2	255	239	7
3	220	207	8
4	558	553	6
5	87	89	18
6	69	56	23
7	108	106	17
8	24	85	44
9	86	30	22
10	404	397	8
11	82	81	25
12	367	390	9

-4 10 1

1	-44	12	27
2	496	493	6
3	93	48	17
4	65	56	22
5	283	269	8
6	322	342	7
7	22	76	45
8	317	317	8
9	99	39	20
10	257	273	10
11	90	57	24
12	342	336	9

-4 11 1

1	-31	2	35
2	36	103	34
3	128	83	14
4	501	509	6
5	170	193	11
6	225	210	9
7	100	58	18
8	-73	0	25
9	102	84	20
10	460	455	8
11	-83	22	25

-4 12 1

1	88	90	19
2	425	439	7
3	74	109	23
4	357	355	7
5	39	52	36
6	252	248	9
7	83	35	22
8	249	254	10
9	37	65	40
10	288	268	9
11	198	196	13

-4 13 1

1	294	314	8
2	-20	41	46
3	359	365	7
4	491	478	7
5	23	101	46
6	286	288	9
7	287	292	9
8	31	54	43
9	389	377	8
10	140	114	16

-4 14 1

1	62	67	27
2	235	236	10
3	170	164	12
4	184	181	12
5	618	577	7
6	113	113	19
7	242	230	10
8	-60	4	31
9	-88	11	24
10	130	94	18

-4 15 1

1	256	241	9
2	-72	54	26
3	628	597	7
4	-63	49	29
5	107	25	19
6	101	82	20
7	299	272	9
8	6	58	63
9	349	349	9

-4 16 1

1	213	201	11
2	232	232	11
3	133	99	16
4	109	117	19
5	382	363	8
6	7	40	60
7	98	122	23
8	150	128	15

-4 17 1

1	89	91	23
2	74	10	26
3	271	280	9
4	249	227	10
5	109	84	20
6	181	177	13
7	110	113	20

-4 18 1

1	-29	37	44
2	207	210	12
3	-83	0	24
4	122	134	18
5	157	128	15
6	117	103	19

-4 19 1

1	52	56	33
2	49	72	36
3	67	58	30
4	165	137	14
5	72	59	28

-4 20 1

1	56	61	33
2	164	147	15

-3 0 1

1	2663	2540	30
3	110	63	15
5	107	86	14
7	263	297	9
9	329	346	10
11	220	279	14
13	25	98	61

-3 1 1

1	353	299	5
2	1259	1172	11
3	1201	1213	10
4	338	364	5
5	570	587	6
6	233	266	6
7	277	311	6
8	106	131	14
9	320	312	7
10	198	165	10
11	293	319	9
12	-50	2	34
13	264	269	10
14	126	84	18

-3 2 1

1	911	895	8
2	87	157	13
3	1195	1191	10
4	144	113	8
5	522	534	5
6	400	396	5
7	179	127	8
8	175	179	9
9	179	190	10
10	64	23	25
11	481	460	7
12	297	311	9
13	93	7	22
14	153	131	16

-3 3 1

1	1466	1403	12
2	722	690	6
3	609	584	6
4	1113	1139	9
5	690	691	6
6	333	349	5
7	576	569	6
8	58	47	24
9	534	553	7
10	451	467	7
11	-9	36	58
12	219	210	11
13	163	178	14
14	-34	13	44

-3 4 1

1	282	283	5
2	1288	1307	11
3	684	660	6
4	99	120	11
5	712	679	7
6	593	585	6
7	177	201	9
8	775	763	7
9	46	65	31
10	382	369	7
11	294	294	9
12	301	282	9
13	-48	57	36
14	142	129	17

-3 5 1

1	157	192	8
2	378	369	5
3	277	269	5
4	1553	1560	13
5	210	204	7
6	736	746	7
7	157	190	10
8	216	209	9
9	244	217	9
10	659	623	7
11	74	23	25
12	313	329	9
13	105	9	20

-3 6 1

1	455	455	5
2	1063	1076	9
3	821	825	7
4	148	152	9

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5	160	152	8
6	413	429	6
7	-44	8	28
8	628	669	7
9	42	93	34
10	302	300	8
11	217	213	11
12	189	195	13
13	140	116	16

-3 7 1

1	572	580	6
2	55	47	19
3	679	686	6
4	637	656	6
5	264	258	6
6	235	240	7
7	56	101	25
8	125	162	14
9	330	305	7
10	366	363	8
11	57	2	31
12	152	162	15
13	170	144	14

-3 8 1

1	269	254	6
2	122	94	10
3	653	681	6
4	120	124	11
5	556	557	6
6	118	92	13
7	48	43	29
8	132	91	14
9	237	221	9
10	-66	38	27
11	425	406	8
12	231	211	11
13	85	74	25

-3 9 1

1	488	491	5
2	187	190	8
3	748	723	7
4	146	159	10
5	236	223	7
6	-59	48	24
7	187	166	10
8	67	68	25
9	205	215	11
10	159	146	14
11	219	239	11
12	86	14	24

-3 10 1

1	825	823	8
2	-50	40	23
3	562	561	6
4	106	95	14
5	381	376	6
6	130	60	13
7	-42	11	33
8	-41	87	35
9	313	310	8
10	95	124	22
11	446	434	8
12	133	91	17

-3 11 1

1	506	494	6
2	68	36	20
3	703	712	7
4	150	162	12
5	239	233	8
6	136	143	13
7	142	136	14
8	-71	7	25
9	295	282	9
10	-31	58	44
11	230	244	11
12	70	91	30

-3 12 1

1	271	266	7
2	215	210	9
3	560	541	6
4	91	64	19
5	373	377	7
6	95	53	19
7	151	151	14
8	66	101	28
9	245	249	10
10	176	162	13
11	346	350	9

-3 13 1

1	254	272	8
2	156	127	12
3	380	366	7
4	491	451	7
5	198	194	11
6	91	75	21
7	75	90	25
8	-72	13	26
9	267	234	10
10	274	269	10
11	91	79	24

-3 14 1

1	-69	28	24
2	543	532	7
3	238	251	9
4	-33	33	39
5	178	159	12
6	327	332	8
7	30	9	42
8	499	472	7
9	67	40	28
10	166	210	15

-3 15 1

1	-35	57	38
2	251	225	9
3	85	43	22
4	598	575	7
5	-13	-34	53
6	278	263	9
7	102	122	21
8	-24	14	48
9	53	59	34
10	328	330	9

-3 16 1

1	118	138	18
2	533	516	7
3	132	119	16
4	60	36	29
5	211	200	11
6	175	173	13
7	47	35	35
8	285	296	10
9	-62	38	32

-3 17 1

1	229	219	10
2	22	11	47
3	126	121	17
4	277	251	9
5	49	70	34
6	-65	17	29
7	193	193	13
8	75	38	27

-3 18 1

1	96	95	22
2	215	233	11
3	114	122	18
4	83	70	24
5	126	112	17
6	59	11	31
7	44	7	37

-3 19 1

1	120	103	18
2	68	2	28
3	247	203	10
4	122	94	18
5	125	76	18
6	86	73	24

-3 20 1

1	181	170	13
2	94	55	22
3	91	110	24
4	-112	13	20

-2 0 1

2	681	638	7
4	452	452	6
6	206	141	9
8	1013	996	11
10	294	253	11
12	412	403	10
14	383	390	12

-2 1 1

1	207	193	3
2	-21	7	23
3	88	106	11
4	423	430	5
5	19	127	33
6	846	811	7
7	25	23	32
8	186	168	9
9	-63	54	24
10	524	508	7
11	147	156	14
12	129	129	17
13	126	97	17
14	40	81	41

-2 2 1

1	551	544	5
2	18	48	26
3	364	357	4
4	701	685	6
5	111	107	10
6	622	664	6
7	372	344	5
8	842	838	8
9	379	359	6
10	23	38	44
11	91	97	21
12	300	311	9
13	105	63	20
14	331	335	9

-2 3 1

1	1041	1082	9
2	756	733	6
3	223	212	5
4	510	492	5
5	587	600	6
6	139	135	9
7	661	639	6
8	190	194	8
9	334	331	7
10	466	470	7
11	340	302	8
12	158	185	14
13	230	242	11
14	131	79	17

-2 4 1

1	35	40	21
2	811	851	7
3	1814	1786	15
4	1010	1003	9
5	440	454	5
6	527	519	6
7	66	96	19
8	542	554	6
9	818	849	8
10	-54	29	30
11	523	486	7
12	-24	52	47
13	223	208	11
14	106	97	21

-2 5 1

1	823	762	7
2	79	78	13
3	420	394	5
4	29	34	27
5	1195	1184	10
6	59	3	19
7	1235	1246	11
8	91	48	17
9	572	577	7
10	23	62	45
11	156	197	14
12	107	121	20
13	282	268	9
14	72	50	29

-2 6 1

1	274	294	5
2	96	70	11
3	1578	1545	13
4	-28	3	27
5	328	316	5
6	97	83	13
7	521	500	6
8	177	169	10
9	750	742	8
10	97	102	20
11	352	375	8
12	57	108	32
13	247	234	10

-2 7 1

1	623	633	6
2	249	214	5
3	175	224	7
4	619	617	6
5	290	252	6
6	294	275	6
7	517	508	6
8	275	280	8
9	397	416	7